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FILE LAST UPDATED: 25 Dec 2002 (20021225/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

CAS roles have been modified effective December 16, 2001. Please check your SDI profiles to see if they need to be revised. For information on CAS roles, enter HELP ROLES at an arrow prompt or use the CAS Roles thesaurus (/RL field) in this file.

=> s (infra-red or IR) (S) water (S) ammonia

3960 INFRA

325745 RED

458 REDS

325986 RED

(RED OR REDS)

3517 INFRA-RED

(INFRA(W) RED)

496949 IR

3672 IRS

499630 IR

(IR OR IRS)

1978802 WATER

217897 WATERS

2029097 WATER

(WATER OR WATERS)

154661 AMMONIA

114 AMMONIAS

154720 AMMONIA

(AMMONIA OR AMMONIAS)

L1 116 (INFRA-RED OR IR) (S) WATER (S) AMMONIA

=> s l1 and (calibrat? or reference? or standard?)

113556 CALIBRAT?

313583 REFERENCE?

154004 REF

1443310 REFS

1586369 REF

(REF OR REFS)

1885072 REFERENCE?

(REFERENCE? OR REF)

201387 STANDARD?

363458 STD

68599 STDS

408619 STD

(STD OR STDS)

558924 STANDARD?

(STANDARD? OR STD)

L2 8 L1 AND (CALIBRAT? OR REFERENCE? OR STANDARD?)

=> d l2 ibib abs 1-8

L2 ANSWER 1 OF 8 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 2001:475526 CAPLUS

DOCUMENT NUMBER: 135:217777

TITLE: Tunneling motions and spectra of hydrogen bonded complexes; the ammonia dimer and the water trimer

AUTHOR(S): Van Der Avoird, A. D.; Wormer, Paul E. S.

CORPORATE SOURCE: Institute of Theoretical Chemistry, NSR Center, University of Nijmegen, Nijmegen, 6525 ED, Neth.

SOURCE: NATO ASI Series, Series C: Mathematical and Physical Sciences (2000), 561(Recent Theoretical and Experimental Advances in Hydrogen Bonded Clusters), 129-153

CODEN: NSCSDW; ISSN: 0258-2023

PUBLISHER: Kluwer Academic Publishers

DOCUMENT TYPE: Journal; General Review

LANGUAGE: English

AB Detailed information on the process of hydrogen bond breaking and formation can be obtained from the spectra of mol. clusters in supersonic beams. At the low temps. in such beams the thermal motions are nearly quenched; what remains are the quantum mech. tunneling motions, involving rotations about hydrogen bonds, as well as the breaking and reconstruction of these bonds. Even the small energy splittings assocd. with such tunneling motions can be investigated in detail by high-resoln. spectroscopy. A hierarchy of motions appear in van der Waals complexes and the nuclear motion problem is solved through the Born-Oppenheimer approxn. which allows computation of vibration-rotation-tunneling (VRT) spectra. Within the chem. bound monomers which constitute the complex, the nuclei vibrate with high frequency but, the motions of the monomers as a whole are much slower, as they move in the field of the weak van der Waals forces. This allows an adiabatic sepn. between the intramol. vibrations and the intermol. motions which usually have large amplitudes. In addn. there are often multiple min. in the potential surface with only low barriers between them, consequently the intermol. "vibrations" may look more like hindered rotations or tunneling motions. Clearly, the **std.** calculational methods are not applicable to the intermol. modes in weakly bound complexes. A review with 110 **refs.** of new

methods for the computation of such VRT states of van der Waals complexes is presented and the theor. results obtained for ammonia dimers and water trimers are compared with new exptl. data.

REFERENCE COUNT: 25 THERE ARE 25 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L2 ANSWER 2 OF 8 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 2001:432982 CAPLUS

DOCUMENT NUMBER: 135:28441

TITLE: Method for measuring water concentration in ammonia

INVENTOR(S): Itou, Taizou; Hayashida, Hideki; Kosuge, Yasuhiro; Ishigaki, Fumiyasu

PATENT ASSIGNEE(S): Showa Denko Kabushiki Kaisha, Japan

SOURCE: Eur. Pat. Appl., 13 pp.

CODEN: EPXXDW

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 1106990	A2	20010613	EP 2000-126959	20001208
EP 1106990	A3	20020911		

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO

JP 2001228085	A2	20010824	JP 2000-346044	20001114
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US 2002061594	A1	20020523	US 2000-732712	20001211
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PRIORITY APPLN. INFO.: JP 1999-351585 A 19991210

JP 2000-346044 A 20001114

US 2000-176799P P 20000119

AB Method and app. for measuring a **water** concn. in **ammonia**, comprising using **ammonia** having a **water** concn. of 10 ppm or less as a **ref.** gas, introducing the **ammonia** at a const. flow rate into a multi-reflection long optical path gas cell, and measuring **IR** absorption intensity of **water** at at least one measurement wave no. in the range of from 3,500 to 4,000 cm⁻¹, from 2,600 to 3,100 cm⁻¹, or from 1,900 to 2,400 cm⁻¹ at which **IR** absorptions of **ammonia** and **water** do not overlap. According to the present invention, anal. of water in a low concn. range of 10 ppm or less in ammonia gas and liquefied ammonia can be performed in a simple and convenient manner. The method is suitable for detn. of concn. of trace water contained in high-purity ammonia used as a raw material in the prodn. of a semiconductor, for example, a GaN-type compd. semiconductor. The method is also suitable for producing ammonia having a decreased water content.

L2 ANSWER 3 OF 8 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 2000:381085 CAPLUS

DOCUMENT NUMBER: 133:81231

TITLE: Optically-pumped far-infrared laser lines in hydrazine, methanol, heavy water, and ammonia: New laser lines and frequency measurements

AUTHOR(S): Vasconcellos, E. C. C.; Allen, M. D.; Zink, L. R.; Evenson, K. M.

CORPORATE SOURCE: Instituto de Fisica, Universidade Estadual de Campinas, Sao Paulo, 13083-970, Brazil

SOURCE: International Journal of Infrared and Millimeter Waves (2000), 21(5), 725-730

CODEN: IJIWDO; ISSN: 0195-9271

PUBLISHER: Kluwer Academic/Plenum Publishers

DOCUMENT TYPE: Journal

LANGUAGE: English

AB A far-IR laser cavity designed to favor short-wavelength laser lines was

used to generate optically-pumped far-IR laser radiation. New far-IR laser lines were discovered in hydrazine, D₂O, NH₃, and several short-wavelength lines previously discovered in MeOH were obsd. Wavelength, frequency, and relative intensity measurements were performed on laser lines in the wavelength range 42.4 to 253.7 μm . Each far-IR frequency measurement was obtained by mixing the far-IR radiation with radiation from 2 **ref.** CO₂ lasers and from a microwave synthesizer in a metal-insulator-metal diode. The pump laser was a high-Q Fabry Perot resonator oscillating on 275 grating-selected laser lines including regular, sequence, and hot band lines.

REFERENCE COUNT: 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L2 ANSWER 4 OF 8 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 2000:347394 CAPLUS

DOCUMENT NUMBER: 133:65744

TITLE: A three-diode-laser, terahertz-difference-frequency synthesizer and its applications toward far-infrared spectroscopy of ammonia and water

AUTHOR(S): Chen, Pin; Pearson, John C.; Pickett, Herbert M.; Matsuura, Shuji; Blake, Geoffrey A.

CORPORATE SOURCE: Time and Frequency Division, National Institute of Standards and Technology, Boulder, CO, 80303, USA

SOURCE: OSA Trends in Optics and Photonics Series (2000), 31(Advanced Semiconductor Lasers and Their Applications), 103-105

CODEN: OTOFZ; ISSN: 1094-5695

PUBLISHER: Optical Society of America

DOCUMENT TYPE: Journal

LANGUAGE: English

AB A solid-state, high-resoln., frequency-calibrated THz spectrometer is presented based on the THz optical heterodyne conversion (TOHC) in low-temp.-grown GaAs using distributed Bragg reflector lasers. The exptl. setup is depicted and described. Spectroscopical investigations were carried out with such a spectrometer for 14NH₃ in the $\nu_2 = 1$ state and for H₂16O in the ground and the $\nu_2 = 1$ state. Twenty-six ν_2 -NH₃ pure inversion and inversion-rotation transitions were measured with a 20 times higher accuracy than for previously published values. Six rotational transitions of H₂O were measured in the ground state and 11 ones in the ν_2 state.

REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L2 ANSWER 5 OF 8 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1999:591417 CAPLUS

DOCUMENT NUMBER: 131:222691

TITLE: Absorption spectrometry of trace moisture in ammonia gas with a 1371 nm distributed-feedback diode laser

AUTHOR(S): Wu, Shang-Qian; Masusaki, Hiroshi; Kimishima, Tetsuya; Kuze, Hiroaki; Takeuchi, Nobuo

CORPORATE SOURCE: Tsukuba Laboratories, Nippon Sanso Corporation, Tsukuba, 300-2611, Japan

SOURCE: Japanese Journal of Applied Physics, Part 1: Regular Papers, Short Notes & Review Papers (1999), 38(8), 4788-4793

CODEN: JAPNDE; ISSN: 0021-4922

PUBLISHER: Japanese Journal of Applied Physics

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The authors report on the sensitivity improvement of in the quant. measurement of trace moisture in ammonia gas. A 1371 nm InGaAsP distributed-feedback diode laser operating at room temp. was used as the light source. A dual-cell optical configuration was employed in the scheme of tunable diode laser absorption spectrometry. Using signal and

ref. cells, both 92 cm in length, the interfering effects of absorption lines of the major constituent gas (ammonia) were canceled in a remarkable manner. Other common mode noises including the etalon fringes assocd. with the wavelength scan were also reduced. The system is capable of detecting trace moisture content of .gtoreq.12 ppb. This is an improvement of more than two orders of magnitude compared with the conventional method of single-cell detection.

REFERENCE COUNT: 31 THERE ARE 31 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L2 ANSWER 6 OF 8 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1996:161915 CAPLUS

DOCUMENT NUMBER: 124:272936

TITLE: Progressive cation solvation at Pt(111) model electrochemical interfaces in ultrahigh vacuum as probed by infrared spectroscopy and work-function measurements

AUTHOR(S): Villegas, Ignacio; Weaver, Michael J.

CORPORATE SOURCE: Dep. Chem., Purdue Univ., West Lafayette, IN, 47907, USA

SOURCE: Electrochimica Acta (1996), 41(5), 661-73
CODEN: ELCAAV; ISSN: 0013-4686

PUBLISHER: Elsevier

DOCUMENT TYPE: Journal; General Review

LANGUAGE: English

AB The utility of IR reflection-absorption spectroscopy (IRAS) for exploring ionic solvation at model electrochem. interfaces in ultrahigh vacuum (uhv) is briefly reviewed with 52 refs. and illustrated for the specific cases of K⁺ solvation by water, methanol, acetonitrile, acetone, and ammonia on Pt(111). The solvents were selected so to span a range of physicochem. properties, while K⁺ is an alkali cation typical of conventional electrochem. double layers which can reliably be dosed (as K atoms) to yield known low coverages on Pt(111). Along with the IR spectra, changes in the surface work function (.DELTA..PHI.) are evaluated for progressive solvent dosages onto both clean and K⁺-predosed Pt(111), both as a means of exploring the solvation-dependent interfacial potential profile and also to provide the required link between the uhv-based and electrochem. potential scales. In each case, low solvent dosages onto K⁺-predosed Pt(111) yielded IR spectra for intramol. solvent modes, esp. for dipolar functional groups, which are markedly different from those obtained on the clean surface, and consistent with the occurrence of progressive cation solvation. Analyses of solvent dosage-band intensities as well as frequencies enable solvent structures within the primary, and in some cases secondary, solvation shell to be suggested. The important role of the metal surface in modifying the nature of such cation solvation is intriguingly evident upon comparing the present IRAS data with corresponding vibrational spectra for progressive solvation of alkali-metal cations by methanol and ammonia in the gas phase. The .DELTA..PHI. responses to solvent dosage in the presence of predosed K⁺ are typically non-monotonic, and feature significant initial .PHI. increases which are consistent with cation-induced solvent reorientation. The marked .PHI. decreases uniformly obsd. for the solvents dosed onto unmodified Pt(111), however, do not correlate simply with the solvent orientation as deduced by IRAS. Some more general implications of such combined IRAS/work-function measurements for exploring double-layer structural issues are pointed out.

L2 ANSWER 7 OF 8 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1993:179012 CAPLUS

DOCUMENT NUMBER: 118:179012

TITLE: Molecular interactions and hydrogen bond tunneling dynamics: some new perspectives

AUTHOR(S): Saykally, Richard J.; Blake, Geoffrey A.

CORPORATE SOURCE: Dep. Chem., Univ. California, Berkeley, CA, 94720, USA

SOURCE: Science (Washington, DC, United States) (1993),
259(5101), 1570-5
CODEN: SCIEAS; ISSN: 0036-8075
DOCUMENT TYPE: Journal; General Review
LANGUAGE: English

AB A review with 38 **refs.** The recent development of tunable far-IR lasers and other high-resoln. spectroscopic probes of weakly bound clusters is having a significant impact on understanding of intermol. forces and on the complex quantum tunneling dynamics that occur in hydrogen-bonded systems. Far-**IR** studies of a variety of interactions are discussed, including several prototypical **water**-hydrophobe complexes, the **water** trimer, and the **ammonia** dimer. Particular attention is paid to the inversion of spectroscopic data to yield detailed intermol. potential energy surfaces. Investigations of nonpairwise additivity are also described.

L2 ANSWER 8 OF 8 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1990:541079 CAPLUS
DOCUMENT NUMBER: 113:141079
TITLE: The intermolecular vibrations of the ammonia water complex. A matrix isolation study [Erratum to document cited in CA112(6):44619u]
AUTHOR(S): Engdahl, Anders; Nelander, Bengt
CORPORATE SOURCE: Chem. Cent., Univ. Lund, Lund, S-221 00, Swed.
SOURCE: Journal of Chemical Physics (1990), 92(10), 6336
CODEN: JCPSA6; ISSN: 0021-9606
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Errors in the title, text, equations, **ref.** 6, and Tables I and III have been cor. The article deals with the intermol. vibrations of the ammonia water complex, not intramol. vibrations as originally reported. The errors were reflected in the abstr. and index entries.